

1,4-Dioxane
123-91-1 | DTXSID4020533

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -12.0 °C

Global applicability domain: Inside

Local applicability domain index: 7.38e-01

Confidence level: 4.94e-01

Nearest Neighbors from the Training Set

Image not found

1,3-Dioxane

Measured: -45.0

Predicted: -12.0

Image not found

1,4-Dioxane

Measured: 11.8

Predicted: -12.0

Image not found

2-Methoxy-3,4-dihydro-2H-pyran

Measured: 16.0

Predicted: 3.43

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1,3-Dimethoxybenzene

Measured: -52.0

Predicted: 10.7

Image not found

1,3,5-Trimethoxybenzene

Measured: 54.5

Predicted: 51.0